LA-UR-21-29053
Approved for public release; distribution is unlimited.

Title: Coupled radiation transport and plasma physics for ICF simulations

Author(s): Hammer, Hans Ruediger
Park, HyeongKae
Chacon, Luis
Taitano, William
Anderson, Steven Edward
Simakov, Andrei N.

Intended for: Presentation to external collaborators

Issued: 2021-09-14

Coupled radiation transport and plasma physics for ICF simulations

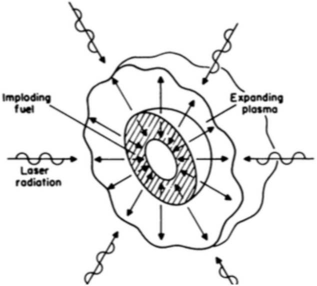
Hans Hammer HyeongKae Park Luis Chacón William Taitano
Steven Anderson Andrei Simakov

March 9, 2021

Motivation

Describing high-temperature plasmas requires inclusion of several nonlinear coupled physics

- Ion kinetics - for each isotope species present in the plasma
- Electron kinetics
- Thermal radiative transfer (TRT)
- Electromagnetic description
- Nuclear reactions (Fusion burn)



TRT is a key physics component in ICF

- Thermal x-ray radiation becomes the dominant energy transfer mechanism in hohlraum
- Driver of capsule implosion
- Radiative energy loss

Scope of this project

Simulating plasmas in ICF hohlraums.

Our project aims to solve

- Kinetic ions (particles)
- Fluid electrons
- Energetic electrons
- Electromagnetics
- Kinetic radiation (MG DP solver)
- Laser-plasma interactions

Coupling of the different physics is done in a nonlinear LO system

- Moment (fluid) equations for plasma
- Gray radiation diffusion
- Consistency terms enforce HO solution
- Concept has been tested in iFP

This presentation describes work done in iFP, which is slightly different

DR project equations - Overview

We try to solve a coupled system with these equations
(missing hot electrons, laser-plasma-interactions):

Ion Vlasov-Fokker-Planck: $\partial_t f_\alpha + \boldsymbol{u}\cdot\boldsymbol{\nabla}_x f_\alpha + \frac{q_\alpha}{m_\alpha}\boldsymbol{E}\cdot\boldsymbol{\nabla}_u f_\alpha = \sum_\beta C_{\alpha\beta}$

Radiation transport: $\frac{1}{c}\partial_t I + \Omega_i \partial_i I + \sigma_t I - \sigma_e B = S_{\boldsymbol{\Omega}'\to\boldsymbol{\Omega},\nu'\to\nu}$

Quasineutrality: $\sum_\alpha q_\alpha n_\alpha + q_e n_e = 0$

Ambipolarity: $\sum_\alpha q_\alpha n_\alpha u_{\alpha,i} + q_e n_e u_{e,i} = 0$

Electron temperature
$$\partial_t \tfrac{3}{2} n_e k_\mathrm{B} T_e + \partial_i u_{e,i}\left[\tfrac{3}{2} n_e k_\mathrm{B} T_e + P_e\right] + \partial_i Q_{e,i} - q_e n_e u_{e,i} E_i - \sum_\alpha W_{e\alpha} - S_{re} = 0$$

Ohm's law: $E_i = \frac{\partial_i P_e + \sum_\alpha F_{\alpha e,i} - S_{rp,i}}{q_e n_e}$

Vlasov-Fokker-Planck equation

Electrostatic kinetic plasma equation with Coulomb collisions

$$\partial_t f_\alpha + \boldsymbol{u}\cdot\boldsymbol{\nabla}_x f_\alpha + \frac{q_\alpha}{m_\alpha}\boldsymbol{E}\cdot\boldsymbol{\nabla}_u f_\alpha = \sum_\beta C_{\alpha\beta}$$

where

- $f_\alpha\left(\boldsymbol{x}, \boldsymbol{u}, t\right)$ velocity distribution function for species α
- $\boldsymbol{E}\left(\boldsymbol{x}\right)$ electric field
- q_α species charge
- m_α species mass
- $C_{\alpha\beta}\left(f_\alpha, f_\beta\right)$ Fokker-Planck collision operator with species β (Rosenbluth et al., 1957)
- $\boldsymbol{\nabla}_x$ gradient operator in physical space
- $\boldsymbol{\nabla}_u$ gradient operator in velocity space

Thermal Radiative Transfer Equation

Thermal radiative transfer (TRT) with physical scattering can be described by the following equation

$$\frac{1}{c}\partial_t I + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}_x I + \sigma_t I_{-}\sigma_e B = \int_0^\infty \int_{4\pi} \sigma_s \left(\boldsymbol{\Omega}' \to \boldsymbol{\Omega}, \nu' \to \nu\right) I\left(\boldsymbol{\Omega}', \nu'\right)\, d\boldsymbol{\Omega}'\, d\nu'$$

where

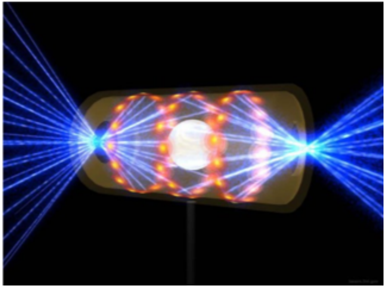
- $I\left(\boldsymbol{x}, \boldsymbol{\Omega}, \nu, t\right)$ Radiation intensity in direction $\boldsymbol{\Omega}$ and frequency ν
- $B\left(\nu, T_e\right)$ Planck function (nonlinear emission spectrum)
- $\sigma\left(\boldsymbol{x}, \rho, \nu, T_e\right)$ Opacity (total, emission, and scattering)

Nonlinearly coupled to electron physics by ρ and T_e. The frequency-integrated emission source is $\propto T_e^4$

Common Approach for Radiation-Plasma coupling

This system is difficult to solve

- Stiff coupling between radiation and material temperature ($\propto T^4$)
- High dimensionality of the transport equation



ICF Hohlraum. Source: LLNL

Common aproaches to solve this

- Linearization of emission-source
- Operator-split temporal update
- Monte-Carlo methods for Boltzmann integral

State of the Art in Plasma-Radiation coupling

Current radiation-hydrodynamics codes use a fluid model for plasma

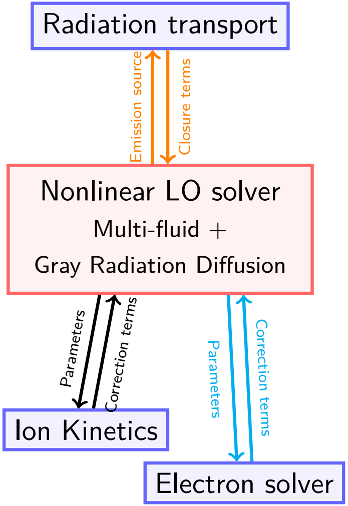
- Plasma described by bulk quantities (moments)
- Assume the plasma is sufficiently collisional (Small Knudsen number)
- Heat flux limiter required to avoid nonphysical behavior

This assumptions are violated in ICF plasmas

- Free streaming of ions and electrons
- Counter-flows
- Non-maxwellian velocity distribution

We need to understand when and where these assumptions are not valid, and the effects

Multi-physics coupling through low-order system



To efficiently couple these equations, we employ a system of low-order (LO) equations

- LO system is tightly coupled
  - Moments of the kinetic equations
  - Implicit time-discretization
  - Solved with non-linear solver (e.g. Newton-Krylov)
- LO-equations are corrected by high-order (HO) solution
  - Example of existing methods: Variable Eddington tensor formulation/ quasi-diffusion
- HO-solvers are (mostly) independent from each other
  - HO-solvers use LO-solution for coupled parameters (e.g., T_e for emission source, u_e for motion correction)

Kinetic electrons have been implemented in a different branch of the iFP code

LO equations - Ions (Moments of VFP)

Conservation of mass (continuity)

$$\partial_t \rho_\alpha + \partial_i \rho_\alpha u_{\alpha,i} + \gamma_{\mathrm{V},\rho,\alpha} - \gamma_{\mathrm{FP},\rho,\alpha} = 0,$$

Conservation of momentum

$$\partial_t p_{\alpha,i} + \partial_j p_{\alpha,i} u_{\alpha,j} + \partial_i P_\alpha - q_\alpha n_\alpha E_i + \sum_\beta F_{\alpha\beta,i} + F_{\alpha e,i} + \gamma_{\mathrm{V},p,\alpha,i} - \gamma_{\mathrm{FP},p,\alpha,i} = 0,$$

Conservation of energy

$$\partial_t U_\alpha + \partial_i u_{\alpha,i} \left[U_\alpha + P_\alpha\right] - q_\alpha n_\alpha u_{\alpha,i} E_i + \sum_\beta W_{\alpha\beta} + W_{e\alpha} + \gamma_{\mathrm{V},U,\alpha} - \gamma_{\mathrm{FP},U,\alpha} = 0.$$

where

- Mass density $\rho_\alpha = m_\alpha n_\alpha$
- Bulk velocity $u_{\alpha,i}$ (Tensor notation)
- Total energy $U_\alpha = 3/2 n_\alpha k_\mathrm{B} T_\alpha + 1/2 \rho_\alpha u_{\alpha,i}^2$
- Friction terms $F_{\alpha\beta}$
- Energy exchange terms $W_{\alpha\beta}$
- Pressure P_α
- Consistency terms γ_V and γ_{FP}

LO equations - Electrons (Hybrid)

The electron number density can be calculated using quasi-neutrality

$$\sum_\alpha q_\alpha n_\alpha + q_e n_e = 0,$$

and the electron velocity using ambipolarity

$$\sum_\alpha q_\alpha n_\alpha u_{\alpha,i} + q_e n_e u_{e,i} = 0.$$

The electron temperature equation is coupled with radiation

$$\partial_t \frac{3}{2} n_e k_\mathrm{B} T_e + \partial_i u_{e,i} \left[\frac{3}{2} n_e k_\mathrm{B} T_e + P_e \right] + \partial_i Q_{e,i} - q_e n_e u_{e,i} E_i - \sum_\alpha W_{e\alpha} - S_{re} = 0,$$

where

- Heat flux $Q_{e,i}$
- Radiation energy deposition S_{re}

LO equations - Electric field (Ohm's Law)

Using the electron momentum equation

$$\partial_t p_{e,i} + \partial_j \left[u_{e,j} p_{e,i} \right] + \partial_i P_e - q_e n_e E_i + \sum_\alpha F_{\alpha e,i} - S_{rp,i} = 0,$$

and assuming $m_e \approx 0 \rightarrow p_{e,i} \approx 0$ to get Ohm's law:

$$E_i = \frac{\partial_i P_e + \sum_\alpha F_{\alpha e,i} - S_{rp,i}}{q_e n_e},$$

with $S_{rp,i}$ the radiation momentum deposition.

The DR will use a generalized version of this electric field including electromagnetic effects, Andrei is working on a rigorous formulation

LO equations - Radiation (Gray Diffusion)

Radiation energy conservation

$$\partial_t E_r + \partial_i F_i + S_{re} = 0,$$

Radiation momentum conservation

$$\frac{1}{c^2}\partial_t F_i + \partial_j P_{r,ij} + S_{rp,i} = 0,$$

where

- Gray radiation energy density $E_r = \frac{1}{c}\int_0^\infty \int_{4\pi} I \, d\Omega \, d\nu$
- Gray radiative flux $F_i = \int_0^\infty \int_{4\pi} \Omega_i I \, d\Omega \, d\nu$
- Radiation pressure $P_{r,ij} = \int_0^\infty \int_{4\pi} \Omega_i \Omega_j I \, d\Omega \, d\nu$

Radiation - Plasma coupling

Radiation and plasma couple through energy and momentum exchange terms.

Energy

$$S_{re} = \sigma_a c E_0 - \sigma_e a c T_e^4 + \frac{\sigma_t}{c} u_{e,i} F_{0,i},$$

Momentum (second term negligible for non-relativistic regimes)

$$S_{rp,i} \simeq \frac{\sigma_t}{c} F_{0,i} + \cancelto{\approx 0}{\frac{u_{e,i}}{c^2}\left(\sigma_a c E_0 - \sigma_e a c T_e^4\right)}$$

Isotropic scattering is hidden in the opacities: $\sigma_t = \sigma_s + \sigma_a$

Radiation is assumed to only interact with electrons. Coupling is dependent on u_e and T_e

Radiation - Material motion correction

Interaction of radiation with moving material require material motion corrections

- Using comoving frame
- Lorentz transformation of radiation quantities
- Emission and scattering (Thompson) are isotropic in comoving frame
- Becomes anisotropic in laboratory frame

Simplified material motion correction for non-relativistic velocities (Morel, 2006):

$$F_{0,i} = F_i - u_{e,i} E_r - u_{e,j} P_{r,ij}$$

$$E_0 \simeq E_r - \cancelto{\approx 0}{2 \frac{u_{e,i}}{c^2} F_{0,i}}$$

$$P_{r,ij} = \mathcal{E}_{ij} E_r \qquad \text{with} \qquad \mathcal{E}_{ij} \simeq \frac{1}{3} \delta_{ij} \quad \text{(Eddington tensor)}$$

Radiation Diffusion Approximation

Neglecting the temporal term in the radiation momentum equation, and with the non-relativistic material motion corrections, we get

$$F_i = -\frac{c}{\sigma_t}\partial_j \mathcal{E}_{r,ij} E_r + u_{e,i} E_r + u_{e,j} \mathcal{E}_{ij} E_r,$$

and a simplified momentum deposition

$$S_{rp} = -\partial_j \left[\mathcal{E}_{ij} E_r\right].$$

Cancellations

Several terms are required to cancel

- Stem from different terms and show up in different equations
- Discretization must match

Radiation-Hydrodynamic asymptotic limit

The previous equations yield the rad-hydro formulation in the highly collisional limit

- Substitute radiation coupling terms and cancel
- The plasma fluid model reduces to Euler equations

Radiation diffusion equation simplifies to

$$\partial_t E_r - \partial_i \frac{c}{\sigma_t} \partial_i \left[\mathcal{E} E_r \right] + \partial_i \left[u_{e,i} \left(1 + \mathcal{E} \right) E_r \right] + \sigma_a c E_0 - \sigma_e a c T_e^4 - u_{e,i} \partial_i \left[\mathcal{E} E_r \right] = 0,$$

which gives with the chain-rule the CRASH equation (Holst et al., 2011)

$$\partial_t E_r - \partial_i \frac{c}{\sigma_t} \partial_i \left[\mathcal{E} E_r \right] + \partial_i \left[u_{e,i} E_r \right] + \mathcal{E} E_r \partial_i u_{e,i} + \sigma_a c E_0 - \sigma_e a c T_e^4 = 0$$

Verification M45 Radiative Shock

Planar Mach 45 shock problem (Lowrie and Edwards, 2008)

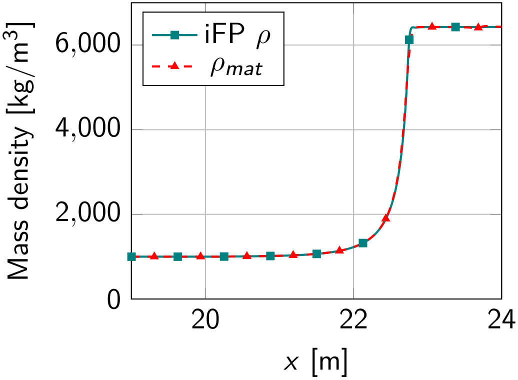
- Shock driven by radiation
- Self-similar solution
- Strongly collisional regime (iFP should reproduce rad-hydro)

Input is for rad-hydro, must be translated to plasma parameters. Special care is required

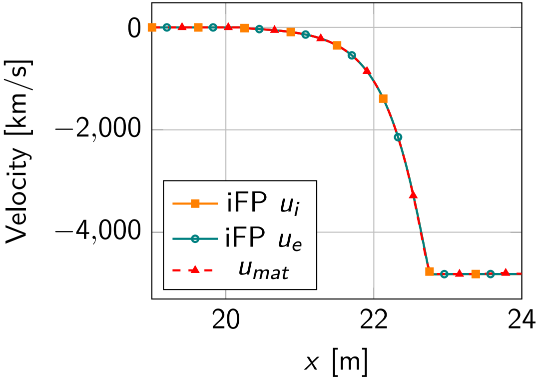
- It looks like a proton (Hydrogen) plasma ($m \approx 1$)
- Rad-hydro input neglected electrons for heat capacity (error)
- To match both heat capacity (sum ions and electrons) and mass density, ion mass must be doubled ($m \approx 2$) (fix)

Special care must be taken for rad-hydro inputs.

Radiative Shock - Results

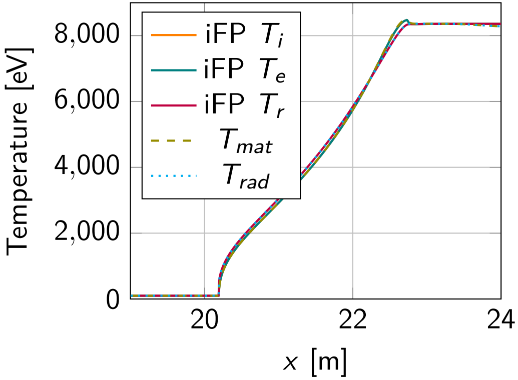


(a) Mass density

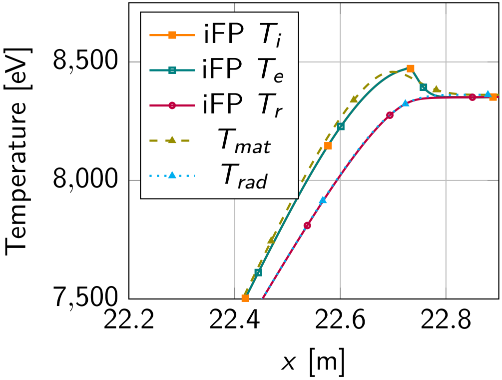


(b) Velocity

Radiative Shock - Results II



(c) Temperature



(d) Temperature at shock peak

Conclusions

Implemented radiation-plasma coupling in the iFP LO solver

- Currently Gray radiation diffusion
- Verified with radiative Mach 45 shock
- Holds in the asymptotic limit

This work is the foundation to ground-breaking improvements

- Extension with HO solver (multi-group diffusion, transport)
- More sophisticated opacity models (tables, LTE, NLTE)

Radiation coupling lessons can be directly translated to DR project

References

- Holst, B. van der et al. (May 2011). "CRASH: A BLOCK-ADAPTIVE-MESH CODE FOR RADIATIVE SHOCK HYDRODYNAMICS—IMPLEMENTATION AND VERIFICATION". In: *The Astrophysical Journal Supplement Series* 194.2, p. 23. ISSN: 0067-0049. DOI: 10.1088/0067-0049/194/2/23.
- Lowrie, Robert B. and Jarrod D. Edwards (July 1, 2008). "Radiative Shock Solutions with Grey Nonequilibrium Diffusion". In: *Shock Waves* 18.2, pp. 129–143. ISSN: 1432-2153. DOI: 10.1007/s00193-008-0143-0.
- Morel, Jim E. (2006). "Discrete-Ordinates Methods for Radiative Transfer in the Non-Relativistic Stellar Regime". In: *Computational Methods in Transport*. Ed. by Frank Graziani. Lecture Notes in Computational Science and Engineering. Springer Berlin Heidelberg, pp. 69–81. ISBN: 978-3-540-28125-2.
- Rosenbluth, Marshall N., William M. MacDonald, and David L. Judd (July 1, 1957). "Fokker-Planck Equation for an Inverse-Square Force". In: *Physical Review* 107.1, pp. 1–6. DOI: 10.1103/PhysRev.107.1.